

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.96e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.37e-01

Confidence level: 3.72e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Molinate</div> <div>Measured: 5.18e-03</div> <div>Predicted: 3.37e-03</div>	<div>Image not found</div> <div>Dichlormid</div> <div>Measured: 2.40e-02</div> <div>Predicted: 4.72e-02</div>	<div>Image not found</div> <div>Furilazole</div> <div>Measured: 7.08e-04</div> <div>Predicted: 7.48e-02</div>
<div>Image not found</div> <div>Phenazone</div> <div>Measured: 2.73e-01</div> <div>Predicted: 1.63</div>		